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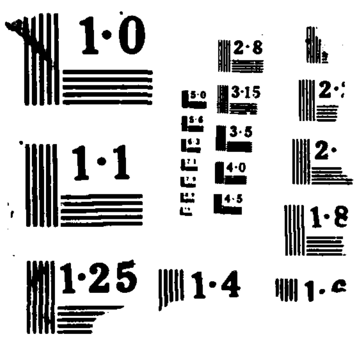
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PROCESS MODEL CONSTRUCTION AND OPTIMIZATION USING STATISTICAL EXPERIMENTAL DESIGN

Emmanuel Sachs and George Prueger

Abstract

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This method has been applied to the development of a model for the low pressure chemical vapor deposition (LPCVD) of polysilicon, a process used in the manufacture of VLSI circuits. A one-dimensional finite difference model of the LPCVD process was constructed. A Taguchi orthogonal array experiment was conducted. A confirming experiment performed at the parameter levels indicated by the Taguchi optimization, served to confirm the validity of the experimental procedure. The experimental results will subsequently be used to calibrate the mechanistic model.

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ABSTRACT

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MOTIVATION FOR PROCESS MODELING

In the most general sense, a process model is a body of knowledge which provides predictions about the outputs from a manufacturing process given information about inputs to the process. Figure 1 illustrates a generic manufacturing process and related processing equipment. The inputs have been divided into usefully distinct categories; process parameters or control factors and noise factors. The process parameters are those parameters that we exercise direct control over. Examples of process parameters include temperature, pressures, roll speeds, gas flow rates, etc. A second set of inputs is entitled disturbances or noise factors. Noise factors are inputs to the process which are subject to unintended and undesired variation. Examples of noise factors include variations in the properties of incoming raw material, and in the process parameters themselves. The goal of the process model is to provide information about the output from the process given information about the process parameters and the noise factors.

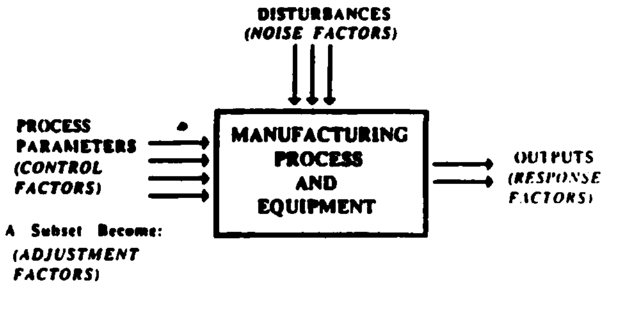


Figure 1. Representation of a Generic Manufacturing Process.

Process modeling has several critical roles to play. A competent model of a manufacturing process is an extremely powerful tool in the design of new processing equipment, as accurate predictive capability will substantially reduce the number of iterations necessary to achieve a satisfactory design.

Process modeling is also essential to the operation of existing equipment. Models can be used to optimize the operation of existing equipment. Optimization might be accomplished by selection of a set of process parameters which leads to the greatest robustness of the process against disturbances or noise factors. Process models are also extremely useful for on-line quality control. While we may think of process optimization as the selection of an operating point for the process, on-line quality control deals with process operation around that operating point. Models can be used to effectively guide the process back to target values.

The construction and utilization of process models is especially critical in modern manufacturing environments. Competitive pressures dictate that processes must be run near their optimum conditions. Computer integrated manufacturing offers a potential wealth of data from process operations which can only be effectively utilized in combination with process models.

APPROACHES TO MODEL CONSTRUCTION

Models may be constructed by three distinctly different approaches; experimental, experiential, and analytical.

Experimentally based process models are constructed by performing deliberate and planned experiments on a process. These experiments are most effectively performed using techniques of statistical experimental design. In these methods such as Box "factorial experimental design and response surfaces" [1, 2] and Taguchi "orthogonal array" [3, 4, 5, 6], many experimental parameters are varied simultaneously in a well-defined plan, resulting in great economy of experimentation. These methods are reviewed briefly in a later portion of this paper.

Experiential process models may be constructed simply by operating the process in production and collecting and analyzing the "observational" or "happenstance" data that results.

Analytical models are based on the fundamental physical mechanisms of the problem. Analytical models can be either closed form, or numerical methods.

Physically based analytical models offer the advantage of having the greatest generality and range of application, however, they can be extremely time consuming to develop, and are often of questionable accuracy and use because of a lack of complete knowledge about the process physics. Experimental and experiential models offer the advantage of good fidelity within the range of variables tested but limited extrapolation capacity beyond that range and limited extension to equipment other than that upon which the experiments were run.

In today's practice, the three methods of model building, experimental, experiential, and analytical, are generally applied independently with little interaction between the methodologies. This papers concerns the fusion of analytical and experimental modeling in order to gain the generality of an analytical model in combination with the precision and ease of use of an experimental model.

BACKGROUND -- DESIGNED EXPERIMENTS

Experimental design is a systematic and organized way to conduct experiments in order to extract the maximum information from the minimum number of experiments. The unifying feature of statistically designed experiments is that all the parameters of interest are varied simultaneously, in contrast to the more conventional one variable at a time experimental technique. In this manner, the total experimental range is explored with a minimum number of experiments. There are two commonly used methodologies for experimental design; the Taguchi orthogonal array method and the Box response surface method.

In the Taguchi orthogonal array method, scientific and engineering knowledge is used to pick experimental parameters which are non-interacting. Typically, three levels would be assigned for each parameter, low, medium and high. The parameters or "control factors" are then arranged in an orthogonal experimental array. Figure 2 shows a four parameter, three level, orthogonal array which defines nine experiments. Also shown in Figure 2 is a graphical representation of the distribution of experimental points for three levels of three control factors or parameters. The points plotted correspond to the second, third and fourth columns of the orthogonal array shown. Such a plot is useful in visualizing the distribution of experimental points in space, but loses its utility past three control factors. The unique feature of an orthogonal array is that for a given level of a given parameter, all other levels of all other parameters are explored uniformly. Thus, for example, in runs one, two and three of the orthogonal array in Figure 2, parameters two, three and four are all rotated through their low, medium and high values.

	Parameters			
Runs	1	2	3	4
1	1	1	1	1
2	1	2	2	2
3	1	3	3	3
4	2	1	2	3
5	2	2	3	1
6	2	3	1	2
7	3	1	3	2
8	3	2	1	3
9	3	3	2	1

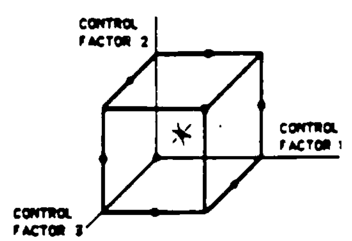
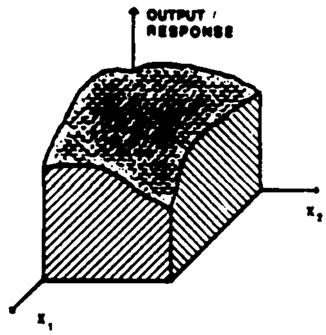


Figure 2. A Taguchi Orthogonal Array and 3 dimensional visualization of columns 2, 3 and 4.

Another unique feature in the Taguchi method is the simultaneous use of "inner" and "outer" arrays. The array shown in Figure 2 is an inner array, and is used to define the points of interest in experimental space. An outer array would be used to define small regions around each of the points specified in the inner array. The outer array would specify, for example, variations or tolerances on experimental parameters or other "noise" factors, thereby defining additional experiments in the neighborhood of each of the nine experiments specified by the inner array.

Perhaps the most distinct feature of the Taguchi method is the interpretation of results by using a "signal to noise ratio". This method of interpretation will be discussed in greater detail later in the paper.

The alternative method, developed by George Box and others, defines a series of experiments and summarizes the results of those experiments in the form of a response surface. A response surface is a polynomial fit (usually a quadratic polynomial) to the measured data. The concept of a response surface and its analytical representation is shown in Figure 3 for a function of two variables, x_1 and x_2. Since the response surface includes the effect of factor interactions, a larger number of experiments is needed to fit a response surface as compared to the Taguchi orthogonal array method. For example, a second degree polynomial fitted to four parameters at three levels, would require a minimum of fifteen experiments as opposed to the nine experiments used in the Taguchi method.



$$\text{RESPONSE} = C_1 + C_2X_1 + C_3X_2 + C_4X_1^2 + C_5X_2^2 + C_6X_1X_2 + \ldots$$

Figure 3. An Illustration of a Box Response Surface.

The response surface method is powerful in its generality, but suffers from the fact that it does not directly embody the sensitivity of the output or response to small deviations of input factors. Since the response surface is a quadratic fit to three points, one cannot expect that the slope at the three points is particularly accurate. Since it is the local slopes that embody the sensitivity information which will be necessary to design a robust process, the quadratic fit response surface is not particularly useful for the design of robust processes.

BUILDING "SMART" RESPONSE SURFACES

The basic conceptual framework of the present work is to replace the polynomial fit of a response surface with a shape dictated by the physics of the process under study. Since the general shape will be dictated by the physics, a more precise model can be obtained with the same number of experimental points, and perhaps even with fewer experimental points. In addition to being more accurate within the experimental range, such a model would also be more useful when extrapolated beyond the tested range.

The remainder of this paper describes one method of constructing such a "smart" response surface. The steps in construction are as follows:

- identify and characterize parameters or factors
- perform designed experiments
- develop a simple analytical model
- calibrate the model
- use the model for a design and operation of equipment

BACKGROUND -- LOW PRESSURE CHEMICAL VAPOR DEPOSITION OF POLYSILICON

The process modeled in this paper is a low pressure chemical vapor deposition process used in the semiconductor industry to fabricate VLSI circuits. Integrated circuits are basically fabricated by alternately depositing and selectively removing layers on a silicon wafer. In the dominant family of CMOS circuits, an individual transistor has three contacts; the source, drain, and gate, as shown in Figure 4 [7]. The most commonly used material for the gate electrode, is polycrystalline silicon, which is deposited on the wafer approximately midway through the fabrication of a CMOS circuit. Polysilicon is used as a conductor at this intermediate fabrication stage, because it allows the wafer to be exposed to subsequent high temperature processing which metallic contacts would preclude.

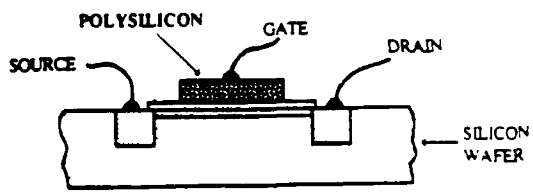


Figure 4. Schematic Cross Section of a MOSFET Transistor.

Polysilicon layers are most commonly deposited on wafers in a batch operation in a tube furnace as shown in Figure 5 [8, 9]. A tube furnace typically consists of a quartz tube surrounded by resisting heating coils which are in turn surrounded by thermal insulation. The four to six inch silicon wafers are held 25 at a time in "boats". Four to six boats are loaded into the tube furnace for each batch. After loading, a partial vacuum is applied to the tube and a process gas in introduced through small tubular "injectors". For low pressure chemical vapor deposition (LPCVD) of polysilicon, the process gas is SiH_4. At the operating temperature of approximately 625° C., SiH_4 pyrolytically decomposes to yield solid silicon which deposits on all hot surfaces, and gaseous hydrogen, according to the relationship:

$$SiH_4 \xrightarrow{625^\circ C} Si + 2H_2$$

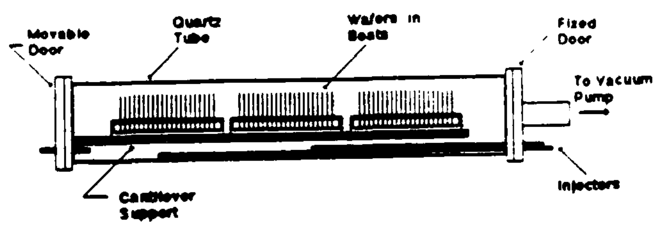


Figure 5. A tube furnace used for the deposition of polycrystalline silicon.

As the reaction proceeds, the liberated hydrogen joins the process gas in the tube, thus diluting the mixture and reducing the reaction rate. It is primarily this dilution which leads to non-uniformities in deposition or growth rate from wafer to wafer down the length of the tube. Wafer to wafer non-uniformity is the primary source of concern in LPCVD of polysilicon. For reasons explained in detail below, across the wafer uniformity tends to be quite good in this process. In order to counteract the SiH_4 depletion and improve the wafer to wafer uniformity in the tube, SiH_4 is introduced or "injected" at three sites in a typical tube furnace as indicated schematically in Figure 5.

Process control is achieved by adjustment of the flowrates through each of the three injectors, adjustment of the axial position of the injectors, temperature adjustment, and control of tube pressure.

IDENTIFICATION AND CATEGORIZATION OF PARAMETERS

The primary control factors or parameters are tube pressure, flowrate through each injector, position of each injector, and temperature profile down the tube.

The possible list of noise factors is quite long, but might prominently include such issues as the amount of prior deposition in the tube, the prior condition of the wafers, aging of the control thermocouples, spacing between the wafers, and location accuracy of the wafers in the tube.

The output or response factor chosen for the current model is the deposition thickness as a function of position down the tube. In practice, one is also concerned with controlling the grain size of the deposition, and the thickness distribution across each wafer. As noted earlier, the thickness across a wafer tends to be quite uniform. As the grain size is controlled almost exclusively by deposition temperature, the desired grain size fixes the temperature of deposition typically at 625° C.

For the purposes of our modeling, we have chosen the four control factors: tube pressure, the flowrate through the load end injector, the flowrate through the center injector, and the position of the source injector. The load end injector is the injector on the left side of Figure 5. The source end injector is the injector whose opening within the tube furnace is furthest to the right in Figure 5. The output or response factor in our experiment will be the profile of thickness down the length of the tube furnace.

EXPERIMENTAL DESIGN, RESULTS, AND INTERPRETATION

The experimental design used was a Taguchi orthogonal array using four parameters at three levels. This array, shown in general form in Figure 2, is again shown in Figure 6 complete with parameter assignments and level selections. Three of the four parameters (all but pressure) are indicated in dimensionless form. The nine experiments were conducted with a wafer load of 150 six-inch wafers. Thirteen test wafers were distributed within the 150 wafer load. A baseline experiment was repeated five times in order to gain some information about run to run variability of the process.

Figure 7 shows plots of growth rate (averaged over the test wafer) against position in the tube furnace for runs one and nine of the orthogonal array. These plots are indicative of the range of results obtained. The mean values and standard deviations of each of the thirteen test wafer positions are shown. The mean value has been obtained from a single run of each experiment. The standard deviation was obtained by normalizing the standard deviation for each wafer position in the baseline replicate runs and applying this normalized standard deviation to the nine Taguchi array experiments. The bar charts at the bottom of the plots in Figure 7 schematically indicates the gas flow at each injector site. As m...

be seen, there is a general correlation between local injector volume and growth rate. The system thus seems to have no conspicuous pathologies.

Experiment Number	Pressure (mtorr)	Q_{load} (% of total)	Q_{center} (% of total)	X_{source} (% of tube length from center)
1	200	20	26.7	9
2	200	30	36.7	12
3	200	40	46.7	15
4	250	20	36.7	15
5	250	30	46.7	9
6	250	40	26.7	12
7	350	20	46.7	12
8	350	30	26.7	15
9	350	40	36.7	9

Figure 6. Taguchi Orthogonal Array Experimental design used.
$Q_{load} + Q_{center} + Q_{source} = 150$ stnd cm^3/min.
Process temperature = 625°.

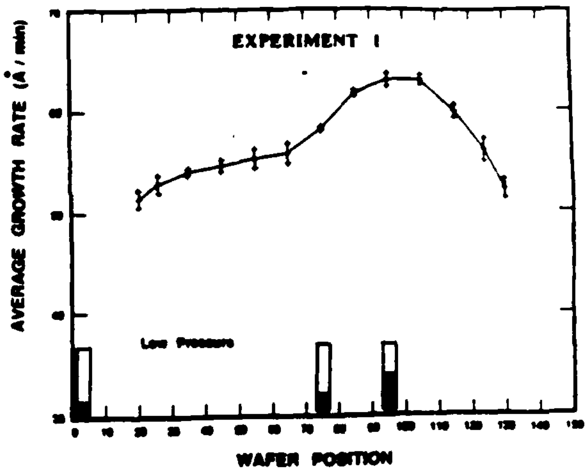
The results of the designed experiments are to be used in two ways. Later they will be used to calibrate the smart response surface model. First, however, they will be used to predict an "optimized" point of operation of the equipment. This predicted optimum will then be run in a confirming experiment. If the resulting improvement is close to that predicted, we may be confident that the experimental parameters and output variables have been properly identified and that the experiments were performed well.

The interpretation of the orthogonal array results is indicated schematically in Figure 8, and begins by calculation of a signal to noise ratio for each of the nine experimental runs. This signal to noise ratio characterizes the deviation of each of the profiles from a flat and uniform profile. Next, average signal to noise ratios are calculated for each level of each parameter, and are plotted on the marginal graphs of Figure 9. These graphs may now be used to select the best combination of parameter levels for an optimized process. This optimum occurs at middle values for load injector, flow source injector, low values for flow source injector position and pressure.

This combination of parameters may now be run in a confirming experiment, the results of which are shown in Figure 10. As may be seen, the confirming experiment is a substantial improvement, thus validating the experimental procedure.

DEVELOPMENT OF THE ANALYTICAL MODEL

The development of the analytical model begins by performing order of magnitude calculations in order to identify important physical mechanisms. First, mass transport calculations indicate that the the deposition rate is limited by the surface reaction rate, and not by transport to the surface. The flow in the annular region between wafers and tube is characterized by a Reynold's number of approximately one, indicating that the flow is laminar. The Peclet number in the annular region is approximately one, indicating that convective and diffusive fluxes are roughly comparable, and that both must be considered in the solution to the problem. A Poiselle flow calculation in the annular space indicates that the pressure drop down the length of the tube is less than one percent of the actual pressure in the tube, and hence is negligible.



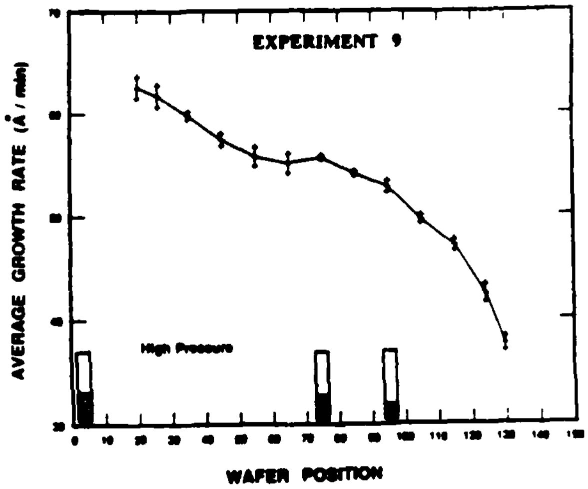
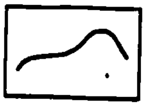


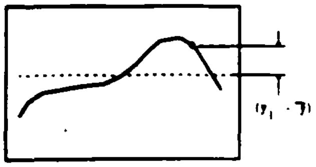
Figure 7. Measured growth rate plotted against temperature for two of the nine experiments defined in Figure 6.

In the region between wafers, the Peclet number is much less than one, indicating that diffusive fluxes dominate, and that the convective flow in this region can be ignored. The exit velocity from the small diameter injector tubes is on the order of 0.5 Mach 1, and hence, the flow geometry and incorporation into the tube annular space is quite complex. The gas depletion, that is the percentage of SiH_4 that is reacted to form silicon, is between 20% and 50%, and is thus, an important component of the problem. Indeed, it is this depletion that is the primary source of the variation in deposition rate. The surface reaction rate is a function of the local partial pressures of SiH_4 and hydrogen and the local temperature.

Consistent with these order of magnitude calculation, our model assumes a one dimensional finite difference formulation with no radial non-uniformities. The flow has been assumed to be inviscid, and to be of a plug flow nature. We are concerned with the coupled problem of convection and diffusion in the annular space. We will consider the thermal problem to be separated from the flow problem and will specify the wafer temperature as a function of position down the tube. We will also specify the annular flow area as a function of position down the tube. We will model the injector flow as mixing into the annular space in the tube over a tube length that is proportional to the square of the flowrate (and velocity) in the tube.

Runs	Parameters 1	2	3	4	S/N
1	1	1	1	1	23.01
2	1	2	2	2	27.55
3	1	3	3	3	18.61
4	2	1	2	3	21.91
5	2	2	3	1	20.89
6	2	3	1	2	23.24
7	3	1	3	2	24.23
8	3	2	1	3	24.79
9	3	3	2	1	17.30





$$S/N = 10 \log_{10}\left(\frac{\text{Mean}^2}{\text{Variance}}\right)$$

$$\text{Variance} = \frac{\sum_{i=1}^{n}(y_i - \bar{y})^2}{n-1}$$

Figure 8. The experimental results are interpreted by calculating a signal to noise ratio for each of the nine experiments of the orthogonal array.

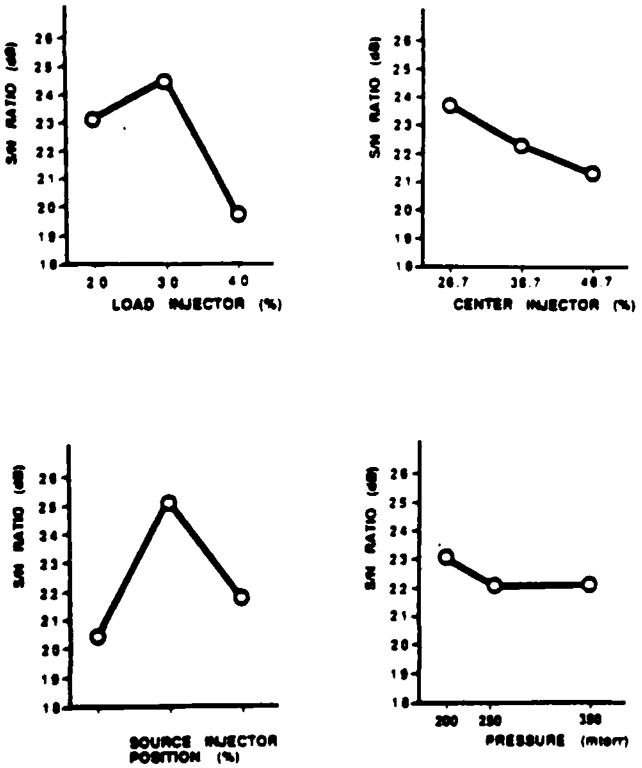


Figure 9. The "marginal graphs" which plot average signal/noise ratio for each level of each parameter.

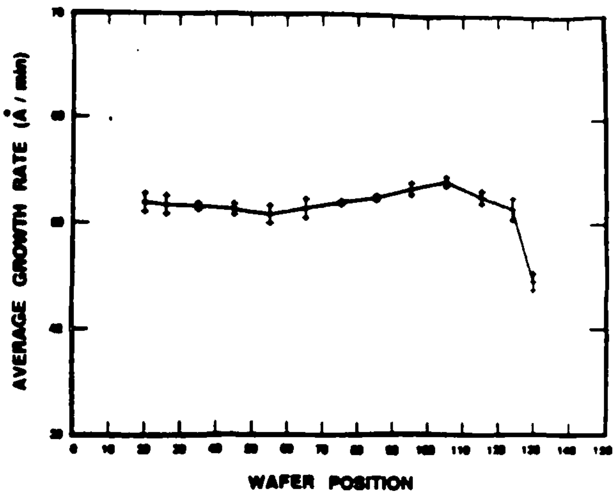


Figure 10. Confirming experiment at "optimized" control factors.

The model basically consists of mass conservation conditions for each of the two species, SiH_4 and hydrogen taken individually and together as summarized in the equations below.

Mass Conservation of Silane:

$$\frac{d}{dz}\left(AcD\frac{dx_s}{dz} - AcV\,x_s\right) = R(x_s) - F$$

Mass Conservation of both species:

$$\frac{d}{dz}(c\,A\,V) = R(x_s) + F$$

where:

A is the cross sectional area of the flow [cm^2],
C is the total concentration of gaseous species [moles/cm^3],
z is the distance down the tube [cm],
D is the diffusion of silane [cm^2/sec],
x_s is the molar fraction of silane [moles/mole],
V is the molar average velocity [cm/sec],
R is the surface reaction rate and is a function of x_s and temperature, [mole/sec · cm],
F represents the injector inlet flow [mole/sec · cm]

MODEL CALIBRATION

The final step in construction of a smart response surface is the use of the results of the experimental design to perform a least squares fit to calibrate the model parameters. The adjustable parameters in our model include four parameters that govern the deposition rate as a function of partial pressures and temperature, and two parameters that specify the nature of the incorporation of injector flow into the annular space.

At the current writing, the model has been developed and found to converge to proper solutions rapidly. In the near future the model will be calibrated using the experimental data.

CONCLUSIONS AND FUTURE WORK

We have illustrated a methodology for the construction of process models using the concept of the "smart" response surface. A smart response surface is one in which the general shape of the response surface is dictated by the process physics and the shape is then calibrated using statistically designed experiments. This approach contrasts with the conventional response surface methods in which a general polynomial is fit to the data derived by designed experiments. The motivation behind constructing a smart response surface is that the resulting model will have greater fidelity in representing the process both within the range of experimentation and when extrapolated beyond the experimental range.

The smart response surface approach has been discussed within the context of building a model for the low pressure chemical vapor deposition of polysilicon as performed in the integrated circuit industry. In the work discussed, a finite difference model of the process was built, and a Taguchi orthogonal array experimental design was performed. The results from the designed experiment were used to optimize the process and a confirming experiment at the predicted optimum conditions demonstrated the validity of the experimental program. In the future, the designed experiments will be used to calibrate the numerical model.

Future work will focus on ways to combine designed experiments with fragmentary mechanistic modeling. This will permit the use of the smart response surface technique without the requirement that a complete physical model be available.

REFERENCES

1. Box, G., Hunter, W., Hunter, J., Statistics for Experimenters, and Introduction to Design Data Analysis and Model Building, Wiley, 1978.

2. Box, G., Draper, N., Empirical Model-Building and Response Surfaces, Wiley, 1987.

3. Taguchi, G., Introduction to Quality Engineering, Krauss International Publications, White Plains, New York 1986.

4. Taguchi, G. System of Experimental Design: Engineering Methods to Optimize and Minimize Costs Vol. 1, Kraus International Publications, White Plains, NY.

5. Phadke, M., Kucjar, N., Speeney, D., and Grieco, M., "Off-Line Quality Control in Integrated Circuit Fabrication Using Experimental Design". The Bell System Technical Journal, 1983.

6. Nackar, R., Shoemaker, A., "Robust Design: A Cost-Effective Method for Improving Manufacturing Processes", AT&T Technical Journal, March/April 1986.

7. Senturia, Stephen D., Wedlock, Bruce D., Electronic Circuits and Applications, John Wiley & Sons, New York.

8. Wolf, Stanley, and Tauber, Richard. Silicon Processing for The VLSI Era, Volume 1: Process Technology, Lattice Press, Sunset Beach, California.

9. Sze, S. M., VLSI Technology, McGraw-Hill Book Company, New York.

10. Jensen, K.F. and Graves, D.B., "Modeling and Analysis of Low Pressure CVD Reactors", J. Electrochem Soc.: Solid-State Science and Technology, September 1983.

11. Van Den Brekel, C.H. and Bollen, L.J.M. "Low Pressure Deposition of Polycrystalline Silicon from Silane", Journal of Crystal Growth 54, 1981.

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